Unifying parameter learning and modelling complex systems with epistemic uncertainty using probability interval

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Abstract

Modeling complex dynamical systems from heterogeneous pieces of knowledge varying in precision and reliability is a challenging task. We propose the combination of dynamical Bayesian networks and of imprecise probabilities to solve it. In order to limit the computational burden and to make interpretation easier, we also propose to encode pieces of (numerical) knowledge as probability intervals, which are then used in an imprecise Dirichlet model to update our knowledge. The idea is to obtain a model flexible enough so that it can easily cope with different uncertainties (i.e., stochastic and epistemic), integrate new pieces of knowledge as they arrive and be of limited computational complexity.

Keywords: Dynamic credal networks, imprecise probability, Dirichlet model, knowledge integration, uncertainty, modelling.

1. Introduction

Firms and industrials of all sectors have to face up new challenging situations. On the one hand, citizens as well as public authorities have stronger demands in terms of quality, safety, ... and on the other hand, they must adapt to the increase of population, global warming and the depletion of fossil resources. This means, among other things, that industrial projects have to integrate sustainability from local to world scale in their conception. Possessing adequate tools to model their systems is likely to make the task easier.

In order to provide relevant conclusions and recommendations, such tools should be able to integrate as much available knowledge as possible, however heterogeneous it is, both in terms of nature (e.g., qualitative expert knowledge vs statistical data) and quality (different precision or degrees of reliability). Such systems are also complex, meaning that the modeling tool

must be able to cope with different scales (e.g., molecular to macroscopic) and with dynamic, time-varying processes. Current researches rely on the development of mathematical tools [53, 6] capable of helping decision-makers to deal with uncertainties, linked for instance to meteorological variations, to expert reliability, *etc.* To summarize, ideal modeling tools should be able to deal with:

- heterogeneous sources of knowledge (Web, data warehouse, experts, . . .)

- mathematical formalisms used by different disciplines (differential equations, graphs, cognitive maps, . . .)

- various manipulated scales (molecular, cellular, population, . . .)

- different forms of uncertainty [32, 36, 40] (natural randomness, imprecision in expert opinions, data scarcity, vagueness, . . .)

In this paper, we propose dynamic credal networks as a possible answer to these challenging tasks to describe complex dynamical systems tainted with stochastic and epistemic uncertainty. As an extension of dynamic Bayesian networks (DBNs) [51], their network structure provides an intuitively appealing interface for human experts to model highly-interacting sets of variables, resulting in a qualitative representation of knowledge. Stochastic and epistemic uncertainties pertaining to the system are then taken into account by quantifying dependence between variables by means of convex sets of conditional probability distributions. The concept of DCNs makes it possible to combine different sources of information, from qualitative expert knowledge to experimental data.

In this paper, we are specifically interested in the problem of parameter learning for a given network structure (assumed to be known), when faced with heterogeneous knowledge. Indeed, while DCN are very attractive modeling tools, they also come with a number of challenges, such as how to control their computational tractability, or how to combine efficiently and easily various pieces of information. For example, how to combine simulations coming from stochastic differential equations with an experimental database, both offering information for the same parameters? We propose to use an imprecise Dirichlet model [7] as a model of the conditional probabilities, and probability intervals as a common uncertainty model to treat different pieces of knowledge. Once transformed, these information pieces gradually increment the set of prior distributions according to the received knowledge, using the Generalized Bayes rule each time additional information arrives. Lower and upper expected *a posteriori* (EAP) are then used as probability bounds to draw inferences from the network. The combination of information is done through a weighted average, allowing us to weigh the importance of the different sources of knowledge.

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80   Section 2 details the material regarding imprecise probabilities as well
81 as the proposed updating scheme of a given parameter set. We then de-
82 scribe in Section 3 how various common sources of information can be
83 transformed into probability intervals. Section 4 presents how we extend
84 Dynamic Bayesian Networks to sets of conditional probabilities, while Sec-
85 tion 5 illustrates the whole approach on a real-case scenario involving cheese
86 ripening.

87 2. Imprecise probabilities and Dirichlet model

88   Let X be a variable [1] taking its values on the finite set $\mathcal{X} = \{x_1, \ldots, x_n\}$,
89 and $p : \mathcal{X} \mapsto [0, 1]$, $\sum_{x \in \mathcal{X}} p(x) = 1$ be a probability mass function over $\mathcal{X}$.
90 $p(X)$ will denote the vector mass function, while $p(x)$ will denote the value
91 taken by p for $X = x$. Such a mass function defines a measure $P_X(A) =$
92 $\sum_{x \in A} p(x)$ for all $A \subseteq \mathcal{X}$.

93 *2.1. Imprecise probability and credal sets*

94   In general, identifying a single probability modelling our uncertainty
95 about some variable X requires a lot of data and/or knowledge. When such
96 knowledge is not available, a safer option is to model our uncertainty by
97 convex sets of probabilities, often called *credal sets* [47, 61, 2]. A credal
98 set associated with X, denoted $K(X)$, is a convex set of probability masses
99 over $\mathcal{X}$. $K(X)$ represents the uncertainty about the unknown value of the
100 variable X. From $K(X)$ are defined upper and lower probability measures
101 of an event $A \subseteq \mathcal{X}$ as

$$\overline{P_X}(A) = \sup_{p \in K(X)} \sum_{x \in A} p(x), \quad \underline{P_X}(A) = \inf_{p \in K(X)} \sum_{x \in A} p(x). \tag{1}$$

102 and, in particular, for any element $x \in \mathcal{X}$ we will have that the upper and
103 lower probabilities are given by

$$\overline{p}(x) = \sup_{p \in K(X)} p(x), \tag{2}$$

$$\underline{p}(x) = \inf_{p \in K(X)} p(x) \tag{3}$$

104 In a subjectivist tradition, the lower probability $\underline{P_X}(A)$ can be interpreted
105 as the maximal price one would be willing to pay for the gamble which pays
106 1 unit if event A occurs (and nothing otherwise) [61]. $\underline{P_X}(A)$ is therefore a
107 measure of evidence in favour of event A, or in other words how much $K(X)$
108 supports event A, while $\overline{P_X}(A)$ measures the lack of evidence against A.
109 $K(X)$ can also be given a robust interpretation, in which it models imperfect

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[1]We adopt notations similar to those of [2, Ch.9] and [24].

110 knowledge of a precise, possibly frequentist, probability p. A credal set
111 $K(X)$ contains a set $\mathcal{E}xt(K(X))$ of extreme probability masses, always finite
112 in this paper, corresponding to the vertices of $K(X)$. Geometrically, $K(X)$
113 may be equivalently specified by the convex hull (denoted CH) of the set
114 $\mathcal{E}xt(K(X))$, i.e.

$$K(X) = CH\{\mathcal{E}xt(K(X))\}. \tag{4}$$

115 The *vacuous* credal set

$$K_v(X) = \{p(X) : p(x) \geq 0, \ \forall x \in \mathcal{X}, \ \sum_{x \in \mathcal{X}} p(x) = 1\} \tag{5}$$

116 that includes all probability masses over $\mathcal{X}$ plays an important role, as it
117 models total ignorance, and should be the starting point of any model. We
118 refer to Walley [61, Sec. 5.5.] for a discussion about uniform probability
119 distribution not being a good model of ignorance.

120 In this paper, we will also be especially interested in particular credal
121 sets $K(X)$ specified by means of *interval probability*

$$K(X) = \{p(X) : \ p(x) \in [l_x, u_x], \ 0 \leq l_x \leq u_x \leq 1, \ \sum_{x \in \mathcal{X}} p(x) = 1\}. \tag{6}$$

122 Indeed, such credal sets that focus over bounds of singletons have the advan-
123 tage to be easier to manipulate, simulate and represent than general ones,
124 while remaining expressive enough (they include both the vacuous and the
125 precise models). We refer to De Campos *et al.* [11] for a detailed exposition,
126 and will only limits ourselves to necessary elements in this paper.

Example 1. Consider an example with three possibilities $\mathcal{X} = \{x_1, x_2, x_3\}$
(e.g., the working states of a system such as "failing", "degraded function-
ing", "fully functioning"), and assume that previous experiments result in
the following intervals

$$p(x_1) = [0; 0.2], \qquad p(x_2) = [0.3; 0.4], \qquad p(x_3) = [0.4; 0.6].$$

The credal set $K(X)$ is the set of all precise probabilities $P(X) = (p(x_1), p(x_2), (p(x_3))$
within these interval bounds. Here $K(X)$ is a polytope defined by the convex
hull of its four vertices in a three dimensional space:

$$K(X) = CH\{(0, 0.4, 0.6); (0.2, 0.3, 0.5); (0.2, 0.4; 0.4); (0.1, 0.3, 0.6)\}.$$

127 Finding these vertices can be done by using classical tools of convex ge-
128 ometry [39], or by using algorithms proper to a given representation (an
129 Algorithm is provided by De Campos *et al.* [11]). The set $K(X)$ is repre-
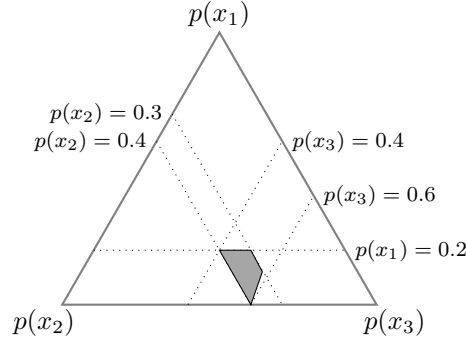130 sented in Figure 1 in barycentric coordinates.

Figure 1: Example 1 credal set in Barycentric coordinates.

2.2. Robust Dirichlet model to learn $K(X)$

An important question is how the credal set $K(X)$ can be instantiated from actual evidence, or in other words how can we go from an initially vacuous knowledge towards a more precise state of knowledge. An instrumental tool to do that is to use a robustified version of the Dirichlet model, also commonly referred to as the Imprecise Dirichlet Model (IDM) [62, 7, 8, 60]. The basic model is based on two hyper-parameters: a positive real value s_0 associated to the strength of prior knowledge, and a vector $\epsilon_0 = (\epsilon_0(x_1), \ldots, \epsilon_0(x_n))$ associated to our initial beliefs about the probabilities of occurrence of elements x_i.

Let $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_n)$ be a vector of chances such that θ_i corresponds to the chance that $X = x_i$. The prior distribution of vectors $\boldsymbol{\theta}$ given by a Dirichlet model is then

$$\text{Dir}(s_0; \xi_0)(\boldsymbol{\theta}) = \frac{\Gamma(s_0)}{\prod_{i=1}^{n} \Gamma(s_0 \xi_0(x_i))} \prod_{i=1}^{n} \theta_i^{s_0 \xi_0(x_i)-1} \tag{7}$$

where Γ is the gamma function. A very easy way to make this model imprecise is to let the vector ϵ_0 become imprecise, and more precisely to consider the set of Dirichlet models

$$\mathcal{M}_{(s_0; \xi_0)} = \{\text{Dir}(s_0; \xi_0)(\boldsymbol{\theta}) : \xi_0 \in \mathcal{T}\} \tag{8}$$

with

$$\mathcal{T} = \{\xi_0 : \ 0 < \xi_0(x_i) < 1 \ , \sum_{i=1}^{n} \xi_0(x_i) = 1\} \tag{9}$$

the open $(n-1)$-dimensional unit simplex. When ξ_0 is precise, the first moments of $\text{Dir}(s_0; \xi_0)$ are given by $E(\theta_i|(s_0; \xi_0)) = \xi_0(x_i)$, and they can be used as estimates of $p(x_i)$, *i.e.*

$$E(\theta_i|(s_0; \xi_0)) = \xi_0(x_i) = p(x_i). \tag{10}$$

6

151 When starting from a vacuous prior knowledge $\xi_0 \in \mathcal{T}$, the bounds over the
152 first moments become

$$\underline{E}(\theta_i|(s_0;\xi_0)) = \min_{\xi_0 \in \mathcal{T}} \xi_0(x_i) = 0 \tag{11}$$

153 and

$$\overline{E}(\theta_i|(s_0;\xi_0)) = \max_{\xi_0 \in \mathcal{T}} \xi_0(x_i) = 1. \tag{12}$$

154 The credal set corresponding to these bounds is then the vacuous one (5).

155 We may then receive additional information from various m sources. A
156 convenient way to encode this information is as a couple $s_k, \mathcal{P}_k, k = 1, \ldots, m$,
157 with $\mathcal{P}_k \subseteq \mathcal{T}$ a convex polytope providing information about the possible
158 chances θ_i, and $s_k \in \mathbb{R}^+$ modelling the strength of the information. We can
159 then update the Dirichlet modelling our uncertainty about $\boldsymbol{\theta}|(s_k;\xi_k)_{k=0}^m$ into

$$\mathcal{M}_{(s_k;\xi_k)_{k=0}^m} = \left\{ \text{Dir}\left((s_k;\xi_k)_{k=0}^m\right)(\boldsymbol{\theta}) : \xi_k \in \mathcal{P}_k \ \forall k \right\}. \tag{13}$$

160 We can then use the posterior first moments to make inferences on chances
161 θ_i

$$\mathrm{E}(\theta_i|(s_k;\xi_k)_{k=0}^m) = p(x_i) = \frac{\sum_{k=0}^m s_k \xi_k(x_i)}{\sum_{k=0}^m s_k} \tag{14}$$

162 As information $\mathcal{P}_k$ are imprecise, we again obtain bounds in the form

$$\underline{E}(\theta_i|(s_k;\xi_k)_{k=0}^m) = \underline{p}(x_i) = \frac{\sum_{k=0}^m s_k \underline{\xi}_k(x_i)}{\sum_{k=0}^m s_k}, \tag{15}$$

$$\overline{E}(\theta_i|(s_k;\xi_k)_{k=0}^m) = \overline{p}(x_i) = \frac{\sum_{k=0}^m s_k \overline{\xi}_k(x_i)}{\sum_{k=0}^m s_k}. \tag{16}$$

163 where

$$\underline{\xi}_k(x_i) = \inf_{\xi_k \in \mathcal{P}_k} \xi_k(x_i) \tag{17}$$

$$\overline{\xi}_k(x_i) = \sup_{\xi_k \in \mathcal{P}_k} \xi_k(x_i). \tag{18}$$

164 These bounds then induce an updated credal set

$$K_{(s_k;\xi_k)_{k=0}^m}(X) = \left\{ p : p(x_i) \in \left[\frac{\sum_{k=0}^m s_k \underline{\xi}_k(x_i)}{\sum_{k=0}^m s_k}, \frac{\sum_{k=0}^m s_k \overline{\xi}_k(x_i)}{\sum_{k=0}^m s_k} \right] \right\} \tag{19}$$

165 that we can use as new knowledge. In practice, s_0 can be interpreted as
166 the number of "unseen" data, and $s_k = s_0$ means that the kth information
167 source has as much importance as our initial uncertainty.

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168   *Remark* 1. The exact updated credal set

$$\tilde{K}_{(s_k;\xi_k)_{k=0}^m}(X) = \left\{ \frac{\sum_{k=0}^m s_k \xi_k}{\sum_{k=0}^m s_k} \; : \; \xi_k \in \mathcal{P}_k, \; \forall k = 1, \ldots, m \right\} \qquad (20)$$

169   is a subset of $K_{(s_k;\xi_k)_{k=0}^m}(X)$, i.e., $\tilde{K}_{(s_k;\xi_k)_{k=0}^m}(X) \subseteq K_{(s_k;\xi_k)_{k=0}^m}(X)$. The set
170   (19) is thus an outer-approximation. Yet, the main advantages of using
171   probability bounds as a basic representation are that

- 172   • their number of extreme points is bounded and relatively low, even
173   when combining them through a weighted average. This is in general
174   not the case if we consider averaging of heterogeneous simple repre-
175   sentations: if we denote $|\mathcal{E}xt(\mathcal{P}_k)|$ the number of extreme points of
176   the kth item of information, then their (Minkowsky) sum $\sum_{k=0}^m s_k \mathcal{P}_k$
177   may have as much as $\prod_{k=0}^m |\mathcal{E}xt(\mathcal{P}_k)|$ extreme points, an exponentially
178   growing number;

- 179   • they are easy to explain and to represent graphically (e.g., as imprecise
180   histograms), therefore offering a convenient way to communicate with
181   domain experts or users not specialized in mathematics or computer
182   science. This is not the case of more complex representations such as
183   belief functions (Section 3.4);

- 184   • except for requiring a finite space, they do not require specific assump-
185   tions, such as the existence of an ordering between elements;

- 186   • they are expressive enough so that they can go from a fully precise
187   probability to the complete ignorance model.

188   None of the other common practical models of information reviewed in Sec-
189   tion 3 have all these advantages at once, making probability bounds a quite
190   convenient model. Given this, using probability bounds seem a good general
191   starting point in applications, not preventing one from investigating refined
192   solutions if the results are unsatisfactory.

193   Of course, in some cases $K_{(s_k;\xi_k)_{k=0}^m}(X)$ may be a poor outer-approximation,
194   however we shall see in Section 5 that it does not necessarily lead to com-
195   pletely void conclusions. Previous studies [1] also suggest that this kind of
196   approximation may be in average reasonable.

197   *Example* 2. Let $\mathcal{X} = \{x_1, x_2, x_3\}$ and $\mathcal{P} = \{\xi : \xi(x_2) \geq \xi(x_1), \; 1/2 \geq$
198    $\xi(x_3), \; \sum_{i=1}^3 \xi(x_i) = 1\}$ be an item of information. The credal set $\tilde{K}_\xi(X)$
199   over $\{x_1, x_2, x_3\}$ obtained by (20) has four extreme points $\{(0, 1, 0), (0, 0.5, 0.5),$
200    $(0.5, 0.5, 0), (0.25, 0.25, 0.5)\}$ that are also extreme points of $K_\xi(X) = \{p :$
201    $p(x_i) \leq \max_{\epsilon \in \mathcal{P}} \epsilon(x_i)\}$. However, the probability $(0.5, 0.25, 0.25)$ is an ex-
202   treme point of $K_\xi(X)$ but not of $\tilde{K}_\xi(X)$.

3. Review of practical sources of information

₂₀₄ Building $K_{(s_k;\xi_k)_{k=0}^m}(X)$ requires to obtain elements of information $\mathcal{P}_k$.
₂₀₅ In this section, we review different practical models and the bounds they
₂₀₆ induce over $\xi_k(x_i)$. We will also provide small examples illustrating what
₂₀₇ kind of information they can model. For the sake of brevity, we will denote
₂₀₈ $\xi(x_i)$ by ξ^i in this section. Note that our information is initially queried on
₂₀₉ observed values x_i, to be then transferred as knowledge on the parameters ξ^i.
₂₁₀ Hence we will consistently refer to knowledge about ξ^i, and to observation
₂₁₁ or information about x_i.

3.1. Precise evaluations

₂₁₃ The most simple models is when the knowledge $\mathcal{P}$ is given by a precise
₂₁₄ vector, in which case $\xi^i = f_i$ is a precise number, and we have

$$\overline{\xi}^i = \underline{\xi}^i = f_i \tag{21}$$

₂₁₅ A classical way to obtain such precise evaluations is when observing $\boldsymbol{m} =$
₂₁₆ $(m_1, \ldots, m_n)$ experiments, where m_i is the number of times x_i was observed.
₂₁₇ In such a case, a classical choice is to take as strength $s = m = \sum_{i=1}^n m_i$
₂₁₈ and $\mathcal{P}$ is the vector $\boldsymbol{f} = (f_1, \ldots, f_n)$ where $f_i = m_i/m$.

₂₁₉ *Example* 3. Assume we can observe three possibilities x_1, x_2, x_3 (e.g., sever-
₂₂₀ ity of a disease, importance of a bacterial population), and we observed 3
₂₂₁ times x_1, 6 times x_2 and one time x_3. We then have

$$f_1 = 0.3, f_2 = 0.6, f_3 = 0.1 \text{ and } s = m = 10 \tag{22}$$

₂₂₂ Note that the more observations we accumulate, the stronger becomes
₂₂₃ this piece of knowledge. s can also be modulated to reflect the reliability
₂₂₄ of data. Note that this model is a degenerated case of probability intervals,
₂₂₅ and can therefore be exactly represented in our framework.

3.2. Numerical possibility distributions and fuzzy subsets

₂₂₇ A possibility distribution π is simply a mapping from $\{\xi^1, \ldots, \xi^n\}$ to
₂₂₈ $[0, 1]$, with at least one element ξ^i such that $\pi(\xi^i) = 1$ [33]. In practice,
₂₂₉ we can see distribution π as an ordering $1 = \pi(\xi^{(1)}) \geq \ldots \geq \pi(\xi^{(n)})$ of the
₂₃₀ elements $x_1, \ldots, x_n$, from the most plausible to the least plausible one.
₂₃₁ Another instrumental way is to encode the possibility distribution through
₂₃₂ the necessity measure N. This necessity measure N is such that

$$N(A_{(i)} = \{\xi^{(1)}, \ldots, \xi^{(i)}\}) = 1 - \pi(\xi^{(i+1)}) \tag{23}$$

₂₃₃ with $\pi(\xi^{(n+1)}) = 0$. $N(A_{(i)})$ can be associated to a lower probability bound
₂₃₄ of event $A_{(i)}$. In particular, the sets $A_{(i)}$ can be interpreted as nested sets
₂₃₅ with an associated lower confidence, these nested sets being built by starting

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236 from the most plausible element $\xi^{(1)}$ and incrementally including the less
237 plausible ones. Note that we may have $\pi(\xi^{(i)}) = \pi(\xi^{(i+1)})$, in which case
238 elements $x_{(i-1)}$ and $x_{(i)}$ would be in the same confidence set.

239   In practice, an expert can provide a possibilistic information by giving
240 confidence bounds over a collection of nested sets. Let $A_1 \subseteq \ldots \subseteq A_m$ be
241 such sets with associated confidence levels $\alpha_1 \leq \ldots \leq \alpha_m$, then it encodes
242 the knowledge $\mathcal{P}_\pi = \{\xi : \sum_{k=1}^{i} \xi^{(k)} \geq \alpha_i, \forall i\}$. From the knowledge on sets
243 $A_1, \ldots, A_m$, one can always come back to an associated distribution π using

$$\pi(\xi^k) = \min_{i : \xi^k \in A_i} 1 - \alpha_{i-1} \tag{24}$$

244 with $\alpha_0 = 0$.

245   Another possibility is to use the formal equivalence between a possibility
246 distribution π and a fuzzy set having π for membership function. This means
247 that an expert conveying information in the form of linguistic assessment [64]
248 can also be modelled by possibility distributions. Deriving bounds on ξ^i from
249 $\mathcal{P}_\pi$ using the possibility distribution π is very easy, as

$$\underline{\xi}^i = 1 - \max_{\xi \neq \xi^i} \pi(\xi) \tag{25}$$

250

$$\overline{\xi}^i = \pi(\xi^i) \tag{26}$$

251 *Example* 4. Assume that an expert is interrogated about the temperature
252 in a room that can be in three states x_1, x_2, x_3. Expert judges that x_2 is
253 the most plausible state, then x_3 and x_1, meaning that $\xi^{(1)} = \xi^2, \xi^{(2)} = \xi^3, \xi^{(3)} = \xi^1$. The expert provides the following confidence values:

$$N(\{\xi^2\}) = 0.5$$

$$N(\{\xi^2, \xi^3\}) = 0.8$$

$$N(\{\xi^2, \xi^3, \xi^1\}) = 1$$

254 which means that the expert has a confidence 0.5 that x_2 will be the observed
255 state, a confidence 0.8 that the observed state will be either x_2 or x_3, and
256 finally is certain that the only observable states are x_1, x_2, x_3. From these
257 values can be deduced the values of the corresponding possibility distribution
258 $\pi(\xi^1) = 0.2$, $\pi(\xi^2) = 1$, $\pi(\xi^3) = 0.5$.

259   Alone, possibility distributions will often be simpler than probability
260 intervals: they require less information (one value per element) and will
261 have a maximal number of $2^{|\mathcal{X}|-1}$ extreme points [56]. Yet the average of
262 multiple sets $\mathcal{P}_{\pi_1}, \ldots, \mathcal{P}_{\pi_m}$ would no longer be a possibility distribution, and
263 the corresponding number of extreme points could explode. Also, possibility
264 distributions cannot model precise probabilities, unless they are degenerate
265 ones.

10

3.3. Probability boxes and clouds

A probability box [35] $\underline{F}, \overline{F}$ is an imprecise cumulative distribution. It can be modelled by two discrete non-decreasing functions $\underline{F}$ and $\overline{F}$ from $(\xi^1, \ldots, \xi^n)$ to $[0,1]$ such that $\underline{F}(\xi^i) \leq \overline{F}(\xi^i)$ for all i in $\{1, \ldots, n\}$ and $\underline{F}(\xi^n) = \overline{F}(\xi^n) = 1$. The values $\underline{F}(\xi^i), \overline{F}(\xi^i)$ are interpreted as the following bounds

$$\underline{F}(\xi^i) \leq \sum_{i=1}^{n} \xi^i \leq \overline{F}(\xi^i)$$

and we can denote by $\mathcal{P}_{\underline{F} \leq \overline{F}}$ the knowledge modelled by a p-box. A p-box information provides us with estimates about the cumulated probabilities of events of the kind $\{x_1, \ldots, x_i\}$, hence assuming that the ordering induced by the indices do make sense.

In the case of p-boxes, the bounds over ξ^i are very easy to determine [59], and are equal to

$$\underline{\xi}^i = \max(0, \underline{F}(\xi^i) - \overline{F}(\xi^{i-1})) \tag{27}$$

$$\overline{\xi}^i = \overline{F}(\xi^i) - \underline{F}(\xi^{i-1}) \tag{28}$$

with the convention $\underline{F}(\xi^0) = \overline{F}(\xi^0) = 0$.

Example 5. Assume we have to assess the how likely it is that a bacterial population is below some threshold, or how likely it is that a component may function for a given period of time. The population sizes or time intervals may be discretized into x_1, x_2, x_3. Assume the following p-box has been given as information

$$\underline{F}(\xi^1) = 0.2, \underline{F}(\xi^2) = 0.7 \text{ and } \overline{F}(\xi^1) = 0.5, \overline{F}(\xi^2) = 0.9.$$

From it we can deduce the bounds

$$\underline{\xi}^1 = 0.2, \underline{\xi}^2 = 0.2, \underline{\xi}^3 = 0.1 \text{ and } \overline{\xi}^1 = 0.5, \overline{\xi}^2 = 0.7, \overline{\xi}^3 = 0.3.$$

P-boxes usually rely on the fact that the set $(\xi^1, \ldots, \xi^n)$ is naturally ordered, and provide confidence bounds over sets of the kind $\{\xi^1, \ldots, \xi^i\}$. However, one possibility is to extend this notion by considering that values ξ^i follows an arbitrary ordering $\xi^{(1)} \leq \ldots \leq \xi^{(n)}$ (for example, from the least to the most plausible element) and to ask to the expert to provide upper and lower confidence bounds about the fact that the truth lies in $\{x_{(1)}, \ldots, x_{(i)}\}$, thus obtaining $\underline{F}(\xi^{(i)})$ and $\overline{F}(\xi^{(i)})$. As in principle any ordering can be used, this is indeed a generalization of p-boxes, known as comonotonic clouds [31]. In particular, in the case where $\underline{F}(\xi^{(i)}) = 0$ for any i, we retrieve the notion of possibility distribution as a special case.

Up to now, what is the maximal number of extreme points of a p-box structure and how to efficiently enumerate them remains an open problem. However, as p-boxes are a special case of belief functions, one can

11

299 use (potentially sub-optimal) algorithms and methods applicable to belief
300 functions [17]. It is also clear that the maximal number of such points is
301 bounded above by the maximal number of extreme point of a belief func-
302 tion ($n!$). Classical p-boxes suffer from the fact that a natural order must
303 exist on $\mathcal{X}$, and when no such order exists, then the average of generalized
304 p-boxes relying on different orders will not be a p-box.

305 *3.4. Belief functions and random sets*

306 Formally, a random set or belief function, initially introduced by Demp-
307 ster [30] and Shafer [57], is defined as a positive mapping $\nu : 2^{\{\xi^1,\ldots,\xi^n\}} \rightarrow$
308 $[0, 1]$ from the power set of $\{\xi^1,\ldots,\xi^n\}$ to the unit interval, such that
309 $\nu(\emptyset) = 0$ and $\sum_E \nu(E) = 1$. From this mapping can then be defined proba-
310 bility bounds $Bel(A), Pl(A)$ for any event that are equal to

$$Bel(A) = \sum_{E, E \subseteq A} \nu(E) \text{ and } Pl(A) = \sum_{E, E \cap A \neq \emptyset} \nu(E) = 1 - Bel(A^c) \quad (29)$$

311 that induce an information $\mathcal{P}_\nu$ such that

$$\mathcal{P}_\nu = \left\{ \xi : \sum_{E \subseteq A} \nu(E) \leq \sum_{\xi^i \in A} \xi^i \leq \sum_{E \cap A \neq \emptyset} \nu(E), \ \forall A \right\} \quad (30)$$

312 In particular, this means that given a function ν, the bounds over elementary
313 events are given by

$$\underline{\xi}^i = Bel(\{\xi^i\}) = \nu(\{\xi^i\}) \quad (31)$$

314

$$\overline{\xi}^i = Pl(\{\xi^i\}) = \sum_{\xi^i \in E} \nu(E) \quad (32)$$

315 Belief functions are instrumental to model frequencies of imprecise observa-
316 tions, for example when multiple exclusive options can be chosen in surveys,
317 or when some sensors sometimes send back imprecise observations. They
318 also include p-boxes, comonotonic clouds and possibilities as special cases.

319 *Example* 6. Assume again that we can meet four different situations x_1, x_2, x_3
320 $, x_4$. Out of 20 observations, x_1, x_2, x_3, x_4 were each perfectly observed re-
321 spectively $3, 2, 5, 6$ times, we observed 3 times the set $\{x_2, x_3, x_4\}$ (excluding
322 x_1) and 2 times the set $\{x_1, x_2, x_3\}$. Such observations can be modelled on
323 $\xi^1, \xi^2, \xi^3, \xi^4$ by the mass

$$\nu(\{\xi^1\}) = 3/20, \nu(\{\xi^2\}) = 2/20, \nu(\{\xi^3\}) = 5/20, \nu(\{\xi^4\}) = 6/20,$$

324

$$\nu(\{\xi^1, \xi^2, \xi^3\}) = 2/20, \nu(\{\xi^2, \xi^3, \xi^4\}) = 3/20.$$

325 From this, we can for example deduce $\underline{\xi}^3 = 0.25$ and $\overline{\xi}^3 = 0.5$.

12

326 Belief functions are general enough to deal with a lot of practical as-
327 sessments, and share the properties of probability intervals that an average
328 of belief functions is still a belief function. However, providing an intuitive
329 graphical representation of a belief function is challenging, and their use may
330 quickly lead to computational issues (e.g., their number of extreme points
331 can be as high as $\mathcal{X}!$ [50])

3.5. Fuzzy random variables

333 Fuzzy random variables have been given different interpretations in the
334 literature, depending on the nature of the fuzzy elements. For example, a
335 fuzzy random variable can be seen as a random phenomenon with precise
336 observations that are fuzzy in nature, or as a random phenomenon with
337 imprecise observations. We refer to [19, 21, 22] for a detailed discussion. In
338 this paper, Fuzzy random variables are interpreted as conditional possibility
339 measures [4, 21], which consist in putting positive masses, not on subsets,
340 but on possibility distributions. They can be modelled by a set $\pi_1, \ldots, \pi_k$
341 where each distribution receives probability mass $p(\pi_i)$. As each π_i can in
342 turn be turned into a mass function ν_{π_i} defined this time over subsets, it
343 is always possible to come back from a fuzzy random variable to a classical
344 mass function, simply by computing for any subset E the value

$$\nu(E) = \sum_{i=1}^{k} p(\pi_i)\nu_{\pi_i}(E).$$

345 We obtain a weighted random sampling of subset E defining a belief function
346 ν. Fuzzy random variables in this context may be cast into the framework
347 of belief functions leading to the same formal advantages and disadvantages
348 of them (see Section 3.4). Fuzzy random variables can result, for instance,
349 from Monte-Carlo simulations of physical models mixing possibilistic and
350 probabilistic uncertainty [4], or from the random observation of fuzzy sets
351 (modelling an ill-calibrated scale, for instance [18]).

3.6. Summary of types of knowledge

353 A final type of knowledge simply consists in directly providing bounds
354 over the values of possible observations x_i. This means specifying, for each
355 ξ^i, the bounds $\underline{f}_i = \underline{\xi}^i$ and $\overline{f}_i = \overline{\xi}^i$. Such bounds are formally equivalent to
356 probability intervals [11].
357 There are multiple ways to derive such bounds: for instance by instan-
358 tiating multinomial confidence intervals over observations, by requiring lin-
359 guistic opinions of the type "probable", "very probable" from the experts
360 and then translating them into numerical evaluations [54], by simply re-
361 quiring numerical evaluations from the experts, when having imprecise his-
362 tograms, . . .

13

363   Table 1 summarises the most common type of practical information one
364 can meet, to what type of information they correspond and how can be
365 computed the lower/upper values $\underline{\xi}^i$ and $\overline{\xi}^i$. These are the values (used as
366 a common mathematical tool) that are then combined and integrated into
367 the learning process developed in Section 2.2.

14

Model	Usual type of information	$\underline{\xi}^i$	$\overline{\xi}^i$
Precise values	Sample/simulation	f_i	f_i
Possibility	Lower confidence on nested sets Linguistic assessments	$1 - \max_{\xi \neq \xi^i} \pi(\xi^i)$	$\overline{\xi}^i = \pi(\xi^i)$
P-boxes and clouds	Lower/upper confidence on nested sets	$\max(0, \underline{F}(\xi^{(i)}) - \overline{F}(\xi^{(i-1)}))$	$\overline{F}(\xi^{(i)}) - \underline{F}(\xi^{(i-1)})$
Belief functions	Imprecise sample	$\nu(\xi^i)$	$\sum_{\xi^i \in E} \nu(E)$
Fuzzy random variable	Fuzzy sample	$\sum_{i=1}^{k} p(\pi_i)\nu_{\pi_i}(\xi^i)$	$\sum_{\xi^i \in E} \sum_{i=1}^{k} p(\pi_i)\nu_{\pi_i}(E)$
Probability bounds	Linguistic assessments Multinomial confidence regions	$\underline{f}_i$	$\overline{f}_i$

Table 1: Summary of the different types of collectible information

4. Robust dynamic probabilistic graphical models

When modeling complex systems, we are not interested in a single variable, but in multiple variables interacting with each others and evolving over time. In theory, our knowledge about these variables, their interaction and evolution can be represented by a credal set defined over the Cartesian product of the corresponding spaces.

In practice, we need tool to represent these interactions, and to simplify the daunting task of specifying a full joint model. Credal networks are graphical (directed) models that aims at encoding our knowledge about variable interactions and at splitting the full joint into multiple, simple conditional models. This section introduces them, as well as their dynamical extension.

4.1. Credal networks

Let $\mathbf{X} = (X_1, \ldots, X_n)$ be a discrete random vector associated with the joint probability mass function $p(\mathbf{X})$ defined over $\prod_{i=1}^{n} \mathcal{X}_i$. Let $K(\mathbf{X})$ be the closed convex set of multivariate probability mass functions describing our knowledge of $\mathbf{X}$.

A credal network (CN) [24, 23] is an extension of Bayesian networks (BNs) where imprecision is introduced in probabilities by means of credal sets [47]. When working with probability sets rather than precise probabilities, the notion of stochastic independence can be extended in several ways [20]. Within graphical models, the most commonly used extension is *strong independence* (also called a *type 1 product* of the marginals in [61]), that induces the strong extension. It can be interpreted as a robust model of a precise yet ill-known BN. Under the *strong extension* [23] hypothesis, the joint credal set $K(\mathbf{X})$ over $\Omega_{\mathbf{X}}$ may be formulated as:

$$K(\mathbf{X}) = CH \left\{ p(\mathbf{X}) : p(\mathbf{X}) = \prod_{i=1}^{n} p_i, p_i \in K_i \right\} \tag{33}$$

where $p_i = p(X_i \mid \mathbf{U}_i)$, $\mathbf{U}_i$ denotes the set of parent nodes of the node X_i and $K_i = K(X_i \mid \mathbf{U}_i)$ is the closed convex set of probability mass function for the random variable X_i given $\mathbf{U}_i$. As mentioned in Section 2, it is sufficient to focus on $\mathcal{E}xt(K(X_i \mid \mathbf{U}_i))$ in Eq. (33).

In this work, we focus on the notion of strong independence and its extension to dynamical models, as this is the most widely used independence notion within graphical models and the one that fits the best with a robust interpretation of probability sets. Other independence notions that may even have asymmetrical versions such as epistemic irrelevance remain computationally intractable [25, 49], except for specific network structures [9] that are usually less complex than the one generally considered here.

16

4.2. Dynamic credal networks

Let $\mathbf{X}(\mathbf{t}) = (X_1(1), \ldots, X_n(1), \ldots, X_1(\tau), \ldots, X_n(\tau))$ be a discrete random vector process associated with the joint probability function $p(\mathbf{X}(\mathbf{t}))$ defined over $\prod_{t=1}^{\tau} \prod_{i=1}^{n} \mathcal{X}_i(t)$. Let $K(\mathbf{X}(\mathbf{t}))$ be the closed convex set of multivariate probability mass functions for $\mathbf{X}(\mathbf{t})$.

A dynamic credal network (CDN) [41] is a dynamic Bayesian network (DBNs) [51] where conditional probabilities $p(X_i(t) \mid \mathbf{U}_i(t))$ (noted p_i^t) are replaced by credal sets $K(X_i(t) \mid \mathbf{U}_i(t))$ (noted K_i^t). It is therefore a time-sliced model that can be used to describe a dynamic process or system[2].

We assume the same *first-order Markov property* as for DBN, meaning that parents only originate from the same or previous time slice, and also that conditional models remain the same at each times slice, that is

$$K(X_i(t) \mid \mathbf{U}_i(t)) = K(X_i(2) \mid \mathbf{U}_i(2)), \ \forall t \in [\![2, \tau]\!]. \qquad (34)$$

Therefore, specifying the graphical structure of a DCN requires the same effort as the one of a DBN (that is, specifying only two consecutive time slices) but allows the user to provide conditional credal sets rather than probabilities if these latter cannot be reliably estimated (from data and/or experts).

4.2.1. Independence in DCN

Extending DBN to DCN requires to specify which kind of independence we consider within and also between each time-slice. We remind that we will only consider extensions relying on the strong independence (33). The most straightforward extension is to simply apply strong independence to the whole network, i.e.,

$$K(\mathbf{X}(\mathbf{t}))_{st} = CH\left\{ p(\mathbf{X}(\mathbf{t})) : p(\mathbf{X}(\mathbf{t})) = \prod_{i=1}^{n} \prod_{t=1}^{\tau} p_i^t, p_i^t \in K_i^t \right\} \qquad (35)$$

We call this extension the *dynamic strong extension* and it is worth noticing that we can have $p_i^t \neq p_i^{t'}$ for $t, t' \in [\![2, \tau]\!]$. That is, we do not assume probabilities within each time-slice to be identical. However, when stepping to dynamic models, Condition (34) allows us to use the notion of *repetitive independence* (also called a *type 2 product* of the marginals in [61]). This condition states that if two variables X, Y have the same set of possible outcomes, that is $\mathcal{X} = \mathcal{Y}$, and can be assumed to be governed by the same probability distribution belonging to $K(X)$, then the joint credal set $K(X, Y)$ is :

$$K(X, Y) = CH\{p(X)p(X) : p(X) \in K(X)\}. \qquad (36)$$

---

[2]It should be noted that the network itself is static, but is used to represent a dynamic process.
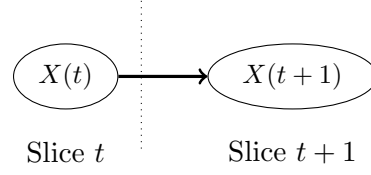
17

Figure 2: A simple dynamical graphical model

Adapting this notion of independence to DCN, so that probabilities of each time slice are assumed to be identical, leads to a second extension, i.e.,

$$K(\mathbf{X(t)})_{rp} = CH \left\{ \begin{array}{l} p(\mathbf{X(t)}) : p(\mathbf{X(t)}) = \prod_{i=1}^{n} \prod_{t=1}^{\tau} p_i^t, \\ p_i^2 \in K_i^2 \text{ and } p_i^t = p_i^2 \; \forall t \in [\![2, \tau]\!] \end{array} \right\} \quad (37)$$

that we call the *dynamic repetitive extension*. We have $K(\mathbf{X(t)})_{rp} \subseteq K(\mathbf{X(t)})_{st}$, as $K(\mathbf{X(t)})_{rp}$ is more constrained. In practice, the strong extension assumes that the dynamic network is ill-defined and that its behaviour can change between time slices, while the repetitive extension assumes that we seek a precise classical DBN who is partially known.

Example 7. Consider the very simple example where $\mathcal{X} = \{0, 1\}$ and the 2-slice network given in Figure 2, which is nothing else than a two-state imprecise Markov chain, and an observed value $X(1) = 1$. Assume furthermore that we have three time slices ($\tau = 3$), that $X(1) = 1$ is observed, and that

$$p(X(t) = 1 | X(t-1) = 0) = 0.8,$$
$$p(X(t) = 1 | X(t-1) = 1) \in [0.2, 0.5].$$

That is, the transition rates from state 0 are precisely known, but not the one from state 1 (although staying in state 1 is clearly less likely). The different extreme points over $(X(1), X(2), X(3))$ resulting from the strong and repetitive extension are summarized in Table 2, in which we adopt the notation $x(t)$ for $X(t) = 1$ for simplification purposes. Each cell of the table corresponds to a precise network obtained by a specific selection of extreme points. The non-specified transition probabilities can be retrieved by the formula $p(X(t) = 1 | X(t-1) = 1) = 1 - p(X(t) = 0 | X(t-1) = 1)$.

4.2.2. Inference algorithms in DCN

(D)CNs can be queried as in (D)BNs to get information about the state of a variable given evidence about other variables, with respect to the chosen network *extension*. However, the use of credal sets makes the updating problem much harder, as it becomes an optimization problem. As such, the computation of the lower bound on $p(\mathbf{X}_Q \mid \mathbf{X}_E)$ requires to minimize a fraction containing polynomials :

18

Strong extension				Repetitive extension			
100	101	110	111	100	101	110	111
$P(x(t)\|x(t-1))=0.5$				$P(x(2)\|x(1))=0.5, P(x(3)\|x(2))=0.2$			
0.1	0.4	0.25	0.25	0.1	0.4	0.4	0.1
$P(x(t)\|x(t-1))=0.2$				$P(x(2)\|x(1))=0.2, P(x(3)\|x(2))=0.5$			
0.16	0.64	0.16	0.04	0.4	0.4	0.1	0.1

Table 2: Simple DCN extreme probabilities

$$\underline{p}(\mathbf{X}_Q(t) \mid \mathbf{X}_E(t)) = \min_{p(\mathbf{X}(\mathbf{t})) \in K(\mathbf{X}(\mathbf{t}))_\omega} \frac{\sum\limits_{X_i(t) \in \mathbf{X}(\mathbf{t}) \backslash \mathbf{X}_Q(t) \cup \mathbf{X}_E(t)} \prod\limits_{i=1}^{n} \prod\limits_{t=1}^{\tau} p_i^t}{\sum\limits_{X_i(t) \in \mathbf{X}(\mathbf{t}) \backslash \mathbf{X}_E(t)} \prod\limits_{i=1}^{n} \prod\limits_{t=1}^{\tau} p_i^t} \qquad (38)$$

with $p(\mathbf{X}(\mathbf{t})) \in K(\mathbf{X})_\omega$ belonging to the *dynamic strong extension* ($\omega = st$) or *dynamic repetitive extension* ($\omega = rp$) of the network. An upper bound can be obtained by maximizing (38). It is known that such a minimum (or maximum) is obtained at a vertex of the *dynamic strong/repetitive extension*. Depending on (1) the structure of network, (2) the number of modality of variables and (3) the chosen extension (strong/repetitive), the updating problem will be more or less complex to solve. Because inferences are already hard in static credal networks, little work has been done on DCNs [41]. By unrolling a two-time slice network over T time steps, the number of possible vertex combinations goes from $\prod_{i,t=0} \#\mathcal{E}xt(K_i^t) \prod_{i,t=1} \#\mathcal{E}xt(K_i^t)$ in the case of repetitive independence, to $\prod_{i,t=0} \#\mathcal{E}xt(K_i^t) \prod_{i,t=1} \#\mathcal{E}xt(K_i^t)^{\tau-1}$ in the case of strong independence. Given the potential number of vertices, approximate algorithms seem more appropriate regarding DCNs.

Many algorithms, exact and approximate, have been proposed to deal with CN. Some are generalizations of well known (D)BNs algorithms. Among the approximate algorithms, there are those that compute inner bounds, i.e. bounds that are enclosed by the exact ones, outer bounds, which enclose the exact ones, and those that perform randomly. The 2U algorithm [34] performs an exact rapid inference in the case of binary tree-shaped (D)CNs with the assumption of *strong independence*. The CCM transformation [15] turns a (D)CN into a (D)BN by adding transparent nodes before performing an Maximum A Posteriori (MAP) estimation over the latter to find the best combination of vertices. It has the same complexity as credal network in-

19

ference, that is $NP^{PP}Complete$, and performs poorly with separately specified credal networks such as the one we used during our trials (because of the sheer number of vertices). Optimization techniques such as branch and bound over local vertices of credal sets [27, 13] are also well suited to medium-sized networks and can be stopped at any time to give an approximate answer. Other algorithms are based on a variable elimination scheme from (D)BNs, such as Separable Variable Evaluation [26, 55] which keeps the separately specified credal sets as separated as possible during propagation, and can be mapped to an integer or a multi-linear program [29, 28]. Regarding binary and DAG-shaped (DAG : Directed Acyclic Graph) credal networks, algorithm L2U (Loopy 2U) [44] (similar to LBP (Loopy Belief Propagation) [63]) produces either inner or outer approximations. Its efficiency is due both to the bounded cardinality of variables and to ignoring loops. Another way to handle credal sets complexity is to represent them by simpler means. Variational methods [43, 42] choose a family of functions to approximate the exact combination of credal sets to decrease computational costs. Those functions are optimized according to some criteria until convergence and the inference is then realized in the network with the original credal sets replaced by the new found functions. The A\R(+) algorithm [27] uses interval probability arithmetic to approximate credal sets in a propagation scheme in tree-shaped networks (with the use of some additional constraints limiting the information loss in its enhanced version). The intervals produced are outer bounds of the real ones. Although those algorithms are fast in medium-sized network, they either produce too many approximations or are too complex to work with DCNs. Another popular family of approximate algorithms producing inner bounds is based on Monte-Carlo sampling [38]. Several methods have been proposed to better guide the search (simulated annealing [12], genetic algorithms [14]) among the vertices of the (conditional) local credal sets, but they require some tuning for more accurate results, otherwise they can lead to poor approximations.

Although there exist several inference algorithms, none allows to do inference, in a realistic and practical way, on networks capable of representing global complex system of Life Sciences. In further inferences, we used a simple Monte-Carlo sampling algorithm [38] which has the advantage to be a good starting point, as it applies with the same easiness to *dynamic repetitive* and *strong extensions* (with a faster convergence for *dynamic repetitive extension*).

4.2.3. Robust parameter learning

Let p_{ijk}^t be the probability that $X_i(t) = x_k$, given that its parents have instantiation[3] x_j (corresponding itself to a vector where j represents the

---

[3]Possible values of variables according to its discretization.

513 vector of parents of i), *i.e.*

$$p_{ijk}^t = p(X_i(t) = x_k | \mathbf{U}_i(t) = x_j) \quad \begin{matrix} i = 1, \ldots, n \\ j = 1, \ldots, c_i \\ k = 1, \ldots, r_i \end{matrix} \quad (39)$$

514 where r_i is the number of values that node i can take and c_i is the number
515 of distinct configurations of $\mathbf{U}_i(t)$. Parameter learning consists in estimat-
516 ing p_{ij}^t faced with available information [45, 10]. For the sake of clarity,
517 parameters p_{ij}^t will be denoted p_{ij} since parameters p_{ij}^t are time-invariant in
518 the case of *repetitive extension* assumption and it is sufficient to only con-
519 sider information limited to each time slice in the case of *strong extension*
520 assumption. According to section 2.2, for all $i \in \{1, \ldots, n\}$; $j \in \{1, \ldots, c_i\}$
521 the credal set $\tilde{K}_{(s_l;\xi_l)_{l=0}^m}(X_i | \mathbf{U}_i = x_j)$ may be approximated by using the
522 outer credal set $K_{(s_l;\xi_l)_{l=0}^m}(X_i | \mathbf{U}_i = x_j)$ defined by

$$K_{(s_l;\xi_l)_{l=0}^m}(X_i | \mathbf{U}_i = x_j) = \left\{ p_{ij} : \ p_{ijk} \in [\underline{p}_{ijk}, \overline{p}_{ijk}], \sum_k p_{ijk} = 1 \right\} \quad (40)$$

523 where $[\underline{p}_{ijk}, \overline{p}_{ijk}]$ is estimated and updated from Eq. (19) according to the
524 available sources of knowledge $(S_0, \ldots, S_m)$.

525 *4.3. Practical robust parameter learning example*

526   Wood is essentially composed of cellulose (denoted C) that is a polymer
527 whose quantity characterizes the nature of wood (denoted T) namely hard-
528 wood or softwood. Imagine that we want to determine the kind of wood
529 according to its chemical composition tainted with uncertainties, that is we
530 are interested in $P(T|C)$. For the sake of clarity, we choose $C = \{x_1 =$
531 $20\%, x_2 = 40\%, x_3 = 60\%\}$ meaning that there is 20%, 40% or 60% of cel-
532 lulose inside wood, $T = \{x_1 = \text{Soft}, x_2 = \text{Hard}\}$ and all sources s_i have the
533 same confidence level, *i.e.* $s_i = 1$ for all i. We thus need to estimate the
534 following parameters:

$$p_{jk} = p(T = x_k | C = x_j) \quad (41)$$

535 according to the available knowledge described in the following. The credal
536 sets $K(T|C = x_j)$ are initialized by

$$K_{s_0}(T|C = x_j) = \{p_{j.} : p_{jk} \geq 0, \sum_k p_{jk} = 1\}, \ \forall j = 1, \ldots, 3 \quad (42)$$

537   1. Precise measures are provided $\{(20, \text{Soft}), (20, \text{Hard}), (40, \text{Hard}), (60, \text{Soft})\}$
538   leading to update by Eq. (19)

539   • $K_{(s_0,s_1)}(T|C = 20) = \{p_{1.} : \frac{1}{4} \leq p_{11} \leq \frac{3}{4}, p_{12} = 1 - p_{11}\}$,

21

540   • $K_{(s_0,s_1)}(T|C = 40) = \{p_{2.} : 0 \leq p_{21} \leq \frac{1}{2}, p_{22} = 1 - p_{21}\}$,

541   • $K_{(s_0,s_1)}(T|C = 60) = \{p_{3.} : \frac{1}{2} \leq p_{31} \leq 1, p_{32} = 1 - p_{31}\}$.

542   2. A first expert says that the more cellulose there is, the harder the
543   wood. This information may be formalized by means of the following
544   fuzzy numbers or possibility distribution (see Section 3.2):

545   • $\pi(T = \text{Hard}|C = 20) = 0.5, \quad \pi(T = \text{Soft}|C = 20) = 1$

546   • $\pi(T = \text{Hard}|C = 40) = \pi(T = \text{Soft}|C = 40) = 1$

547   • $\pi(T = \text{Hard}|C = 20) = 1, \quad \pi(T = \text{Soft}|C = 20) = 0.5$

548   meaning for instance that $P(T = \text{Hard}|C = 20) \leq 0.5$ leading to
549   update

550   • $K_{(s_0,s_1,s_2)}(T|C = 20) = \{p_{1.} : \frac{1}{3} \leq p_{11} \leq \frac{5}{6}, p_{12} = 1 - p_{11}\}$,

551   • $K_{(s_0,s_1,,s_2)}(T|C = 40) = \{p_{2.} : 0 \leq p_{21} \leq \frac{2}{3}, p_{22} = 1 - p_{21}\}$,

552   • $K_{(s_0,s_1,,s_2)}(T|C = 60) = \{p_{3.} : \frac{1}{3} \leq p_{31} \leq \frac{5}{6}, p_{32} = 1 - p_{31}\}$.

553   3. A second expert provides more accurate estimation in terms of confi-
554   dence

555   • $P(T = \text{Soft}|C = 20) \geq 95\%$,

556   • $P(T = \text{Hard}|C = 40) \geq 60\%$,

557   • $P(T = \text{Hard}|C = 60) \geq 95\%$.

558   which can be modeled again by a possibility distribution. This leads
559   to update

560   • $K_{(s_0,...,s_3)}(T|C = 20) = \{p_{1.} : 0.49 \leq p_{11} \leq 0.875, p_{12} = 1 - p_{11}\}$,

561   • $K_{(s_0,...,s_3)}(T|C = 40) = \{p_{2.} : 0 \leq p_{21} \leq 0.6, p_{22} = 1 - p_{21}\}$,

562   • $K_{(s_0,...,s_3)}(T|C = 60) = \{p_{3.} : 0.25 \leq p_{31} \leq 0.64, p_{32} = 1 - p_{31}\}$.

563   4. Defective sensors and measurements provide joint imprecise observa-
564   tions, summarized in Table 3 and producing a joint belief function
565   (Section 3.4).

From this information lower and upper probability bounds over pa-
rameters are given by

$$Bel(T = t|C = c) = \frac{Bel(T = t, C = c)}{Bel(T = t, C = c) + \sum_{t' \neq t} Pl(T = t', C = c)}$$

$$Pl(T = t|C = c) = \frac{Pl(T = t, C = c)}{Pl(T = t, C = c) + \sum_{t' \neq t} Bel(T = t', C = c)}$$

22

	Type		
Focal sets	Soft	Hard	{Soft,Hard}
20	1	2	0
40	4	6	1
60	0	10	1
{20, 40}	10	5	1
{20, 60}	0	0	5
{40, 60}	1	3	10
{20, 40, 60}	0	0	8

Cellulose (row label for the left side of the table)

Table 3: Focal sets occurrences

For example

$$Bel(T = \text{Soft}|C = 20) = \frac{1/68}{1/68 + 21/68} = 0.045$$

$$Pl(T = \text{Soft}|C = 20) = \frac{24/48}{24/48 + 2/48} = 0.926$$

566   Credal set $K_{(s_0,...,s_4)}$ is then updated by

567   • $K_{(s_0,...,s_4)}(T|C = 20) = \{p_{1.} : 0.4 \leq p_{11} \leq 0.89, p_{12} = 1 - p_{11}\}$,

568   • $K_{(s_0,...,s_4)}(T|C = 40) = \{p_{2.} : 0.021 \leq p_{21} \leq 0.65, p_{22} = 1 - p_{21}\}$,

569   • $K_{(s_0,...,s_4)}(T|C = 60) = \{p_{3.} : 0.2 \leq p_{31} \leq 0.67, p_{32} = 1 - p_{31}\}$.

570 5. Real-life case study

571   To illustrate the feasibility and practical use of our approach in a real
572   case, we have focused on the ripening process of the Camembert type soft
573   mould cheese that represents an ecosystem and a bioreactor difficult to ap-
574   prehend from a global point of view [37, 52]. Based on recent works carried
575   out by Baudrit *et al.* [5]; Sicard *et al.* [48], a simplified sub-structure
576   of dynamic Bayesian networks has been extracted (see Figure 3) provid-
577   ing a qualitative representation of the coupled dynamics of yeast behaviour
578   *Kluyveromyces marxianus* (Km, colony forming unit/g of Fresh Cheese in
579   decimal logarithmic scale) with its lactose substrate (lo, g/Kg of Fresh
580   Cheese) influenced by temperature (T, ^{o}C) inside the ripening chamber and
581   involving odour changes ($Od = \{\text{Fresh,Mushroom,Camembert}\}$).
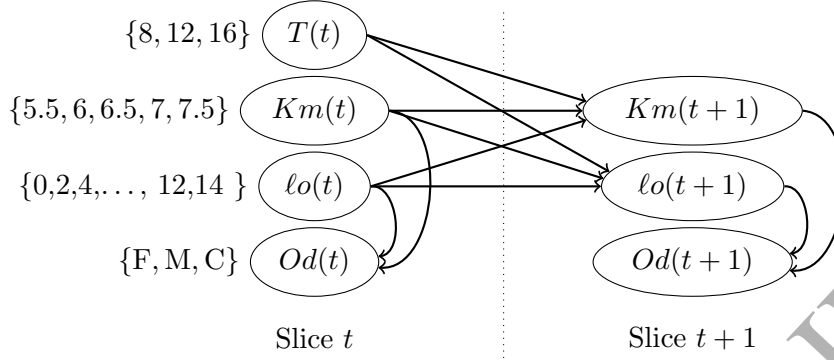
23

Figure 3: Structure of the dynamic credal network and the values of each variables representing the coupled dynamics Km growth versus lo consumptions influenced by temperature involving odour changes during the cheese ripening process (F=Fresh,M=Mushroom,C=Camembert).

5.1. Parameter learning

Assuming *repetitive extension* for computational reason mentioned in Section 4.2.2, we present, in the following, how parameters

$$
\begin{aligned}
\boldsymbol{p_1} &= p(Km(1)), \\
\boldsymbol{p_2} &= p(lo(1)), \\
\boldsymbol{p_3} &= p(T(1)), \\
\boldsymbol{p_4} &= p(Km(2)|(Km(1), lo(1), T(1))), \\
\boldsymbol{p_5} &= p(lo(2)|(Km(1), lo(1), T(1))), \\
\boldsymbol{p_6} &= p(Od(1)|(Km(1), lo(1)))
\end{aligned}
$$

may be estimated by using the robust hybrid parameter learning when we have several sources of knowledge (denoted S_i) tainted with stochastic and epistemic uncertainty.

1. Initialization (S_1).

   All DCN parameters are initialized by:

   - An experimental database $S_{experiments}$ of six cheese ripening trials carried out for temperatures varying from T = 8 to 16 ^oC is available.

   - the vacuous credal sets leading to bracket parameters by [0,1] when no information is available.

   With s_1 corresponding to the confidence level about experimental trials $S_{experiments}$, according to (19) we have:

$$
p_{ijk} \in \left[\frac{s_1 f_{ijk}}{s_0 + s_1}, \frac{s_0 + s_1 f_{ijk}}{s_0 + s_1} \right] \tag{43}
$$

24

where f_{ijk} represents the observed frequency corresponding to sample information in Table 1 and linked to Section 3.1.

2. Integration of partial mechanistic model tainted with uncertainties (S_2). The yeast Km is one of the dominant species in the yeast flora of Camembert cheeses and its principal activity is the consumption of lactose (lo) [46]. Models to determine the growth of microorganisms have been studied in the fermentation industry [58], and the description of the growth of Km is obtained by performing material balances on biomass Km and lactose lo [3]:

$$(S)\begin{cases} \dfrac{dKm}{dt} &= \mu\dfrac{lo}{K_{lo}+lo}Km - b\cdot Km \\ \dfrac{dlo}{dt} &= -\dfrac{\mu}{\beta}\dfrac{lo}{K_{lo}+lo}Km \end{cases} \qquad (44)$$

where μ (the maximum specific growth rate of Km), $K_{lo}(T)$ (the half saturation constant for growth), b (the decay coefficient) and β (the yield coefficient for Km on lactose), depending on temperature, are tainted with stochastic and epistemic uncertainties, due to the natural variability of yeast population and the imperfection of the model. The background knowledge about parameters $\boldsymbol{p_1}$, $\boldsymbol{p_2}$, $\boldsymbol{p_4}$ and $\boldsymbol{p_5}$ are then updated regardless of the rest of network by using a simulated database $S_{simulated}$ resulting from Monte Carlo simulation coupled to interval analysis [4] leading to manage a joint random set $([\underline{Km}(t),\overline{Km}(t)],[\underline{lo}(t),\overline{lo}(t)],T(t))_l$ associated with mass $\nu_l = 1/\#S_{simulated}$ such that for instance

$$p_{4jk} \in \left[\frac{s_1 f_{4jk} + s_2 \underline{\xi}_{4jk}}{s_0 + s_1 + s_2}, \frac{s_0 + s_1 f_{4jk} + s_2 \overline{\xi}_{4jk}}{s_0 + s_1 + s_2}\right] \qquad (45)$$

where

$$\underline{\xi}_{4jk} = \frac{bel(j,k)}{bel(j,k) + \sum_{l\neq k} pl(l,j)} \text{ and } \overline{\xi}_{4jk} = \frac{pl(j,k)}{pl(j,k) + \sum_{l\neq k} bel(l,j)} \qquad (46)$$

and

$$pl(j,k) = \sum_{\substack{l, [\underline{km}(t+1),\overline{km}(t+1)]_l \cap \{km_k\} \neq \emptyset \\ [\underline{km}(t),\overline{km}(t)]_l \cap \{km_j\} \neq \emptyset \\ [\underline{lo}(t),\overline{lo}(t)]_l \cap \{lo_j\} \neq \emptyset \\ T_l(t) = T_j}} \nu_l \qquad (47)$$

25

617 and

$$bel(j,k) = \sum_{\substack{l, \{km_k\} \subseteq [\underline{km}(t+1), \overline{km}(t+1)]_l \\ \{km_j\} \subseteq [\underline{km}(t), \overline{km}(t)]_l \\ \{lo_j\} \subseteq [\underline{lo}(t), \overline{lo}(t)]_l \\ T_l(t) = T_j}} \nu_l \qquad (48)$$

618 This kind information is linked to Sections 3.4, 4.3 and corresponds to
619 Belief functions in Table 1.

620 3. Integration of expert knowledge, (S_3).

621

622 In cheese ripening, as in every complex food process, most of the con-
623 trol measures are performed on the basis of the expert's sensory per-
624 ceptions. Indeed, experts have in mind the ripening process that they
625 oversee and they are able to explain part of the complex reactions
626 through their perception of quality changes [16]. Expert elicitation
627 [48] informs us that during the exponential growing of the yeast Km,
628 a characteristic fresh or lactic odour is released. Mushroom odour
629 appears when the concentration of the yeast Km begins to stabilize
630 and typical Camembert odour appears when the population of Km
631 begins to decay. From this qualitative information, general rules may
632 be deduced such as "it is impossible to have a Camembert odour with
633 a weak (*resp.* high) concentrations of Km (*resp. lo*)". That means for
634 several combinations of Km and lo concentrations, likely values about
635 variable $Odour$ may be formalized by means of possibility distributions
636 $\pi_{Odour}(.|Km, lo)$. That is:

- When there is a high (*resp.* weak) concentration of lactose (*resp.* the yeast Km), having a fresh odour is the most plausible state, followed by Mushroom and Camembert odours, which can be formalized as the following possibility distribution:

$$\pi_{Odour}(\text{Fresh}|j) = 1$$
$$\pi_{Odour}(\text{Mushroom}|j) = 0.8$$
$$\pi_{Odour}(\text{Camembert}|j) = 0.2$$

637 where $j = (Km \leq 6.5, lo \geq 8)$.

- When there is a medium concentration of lactose and Km, the Mushroom odour is the most plausible state but we cannot exclude having Fresh or Camembert odours, formalized by:

$$\pi_{Odour}(\text{Fresh}|j) = 0.2$$
$$\pi_{Odour}(\text{Mushroom}|j) = 1$$
$$\pi_{Odour}(\text{Camembert}|j) = 0.2$$

26

638   where $j = (Km = 7, 2 < lo < 8)$.

- When having very weak (*resp.* high) concentration of lactose (*resp.* the yeast Km), the Camembert odour is the most plausible state, followed by Mushroom and Fresh odours, formalized by:

$$\pi_{Odour}(\text{Fresh}|j) = 0.2$$
$$\pi_{Odour}(\text{Mushroom}|j) = 0.8$$
$$\pi_{Odour}(\text{Camembert}|j) = 1$$

639   where $j = (Km > 7, lo < 2)$.

640   Parameter $\boldsymbol{p}_6$ is then updated by using

$$p_{6jk} \in \left[\frac{s_1 f_{6jk} + s_3 \underline{\xi}_{6jk}}{s_0 + s_1 + s_3}, \frac{s_0 + s_1 f_{6jk} + s_3 \overline{\xi}_{6jk}}{s_0 + s_1 + s_3} \right] \tag{49}$$

641   where

$$\overline{\xi}_{6jk} = \pi_{Odour}(k|j) \text{ and } \underline{\xi}_{6jk} = 1 - \max_{l \neq k} \pi_{Odour}(l|j) \tag{50}$$

642   This kind of information is linked to the Section 3.2 and corresponds
643   to possibilistic model in Table 1.

5.2. Inference results and discussion

645   We attempt to estimate the lower and upper mean time evolution of Km,
646   lo and $Odour$ for a temperature control according to the previous parameter
647   learning. That is

$$\underline{E}(X(t)|\mathbf{U}(t)) = \sum_k x_k \underline{p}(X(t) = x_k|\mathbf{U}(t)) \tag{51}$$

648   for the lower bounds where X may be Km, lo, $Odour$; $\mathbf{U}(t) = (lo(0), Km(0)$
649     $, T(0), \ldots, T(t))$ and

$$\underline{p}(X(t) = x_k|\mathbf{U}(t)) = \inf_{p \in K(X(t)|\mathbf{U}(t))} p(X(t) = x_k|\mathbf{U}(t)) \tag{52}$$

650   by assuming $s_0 = s_1 = s_2 = s_3 = 1$ and the *repetitive independence*, since
651   we assume that transition probabilities remain the same along the process
652   (there is no reason to assume a change in the bacteria population behaviour),
653   but are ill-known due to insufficient experiments and information.   Figure
654   4 displays the lower and upper simulated mean evolution of Km, lo, $Odour$
655   versus experimental data over the cheese ripening carried out at 12^oC each
656   time a source of information is added. Supported by Table 4, we may observe
657   that the imprecision of simulated results well decreases (characterized by the
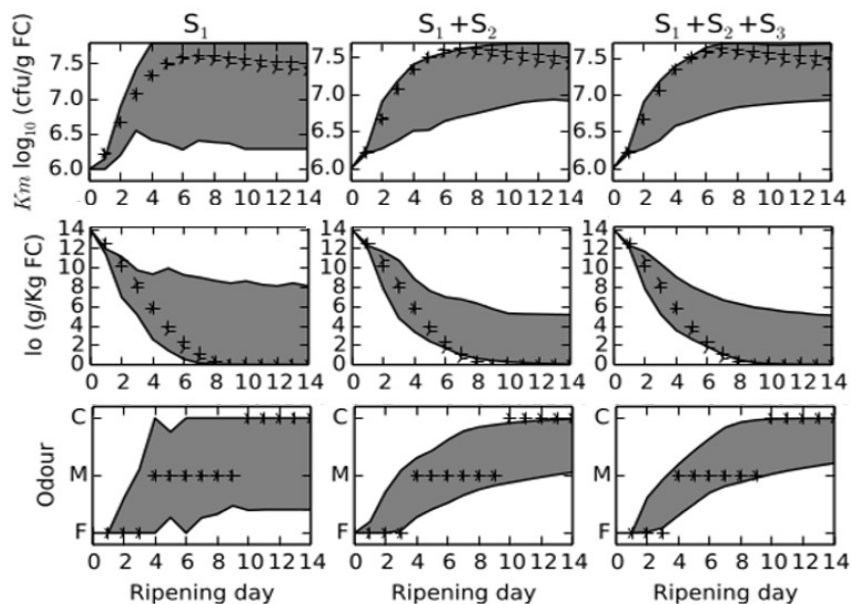658   surface in gray).

27

Figure 4: Incremental DCN average simulation versus raw data (dotted) of Km, lactose (lo) and Odour for a ripening carried out at and T=12° C each time a new source of information is integrated.

	Km	lactose	Odour
Source 1	18.62	105.38	20.91
Source 1 & 2	11.37	71.06	13.77
Source 1& 2& 3	11.03	71.32	10.99

Table 4: Area between the lower and upper bounds of the simulated mean time evolution

28

6. Conclusion

There are complex dynamical processes for which no deterministic model describing the complete process exists. In such cases, dynamic credal networks are convenient models that allow to include expert knowledge, data and variable interaction in a single framework. They allow a faithful representation of incomplete knowledge or scarce data, that are inherent to the complexity of bio-physicochemical phenomena occurring in Life Sciences. In this paper, we attempted to implement a practical methodology coupling interval analysis and Dirichlet model in the framework of dynamical credal networks for building mathematical model capable of representing complex systems. Moreover, the concepts of dynamic repetitive and strong extensions have been proposed. While the latter can be seen as a straightforward extension of classical credal networks, the former considers repetitive independence to allow the model to preserve a temporal regularity. Methodology has been applied to a simplified real-case study concerning microbial population growth involving sensory evolution during cheese ripening. These experiments have shown that including information reduces imprecision about result simulations. Next tools should consider to manipulate, to combine convex sets in order to not lose information during incremental parameter learning. In further works, DCNs should enable us to determine the contribution of imprecision and/or incompleteness on the outcomes of a model in order to know if an ambiguous answer is due to a lack of information or due to a random phenomenon. That is, we plan to develop refined sensitivity analysis techniques based on their use. They should thus determine key variables and/or key phenomena for which it will be necessary to acquire more information. Finally, we also plan to investigate their usefulness in determining optimal commands.

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₈₇₉ **Vitae**

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